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The work supported by this Contract focuses on the fundamental processes involved in spray combustion, transition to detonation, flame-acoustic interaction and vapor explosions. These processes include single-phase and multi-phase fluid dynamics, thermodynamics and chemical kinetics. The interactions and couplings among these processes have been of particular interest.

The research effort in multiphase dynamics includes an examination of the entropy inequality to see if it can provide constraints on constitutive equations; derivation of constitutive equations for high Reynolds number flow of spherical droplets; derivation of a model for the evolution of geometric parameters during the flow; and derivation of a model for particle velocity fluctuations in a fluid.

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Flow and Chemical Reaction in Homogeneous and Heterogeneous Media

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Prepared by D. A. Drew and A. K. Kapila

Research

The work supported by this Contract focuses on the fundamental processes involved in spray combustion, transition to detonation, flame-acoustic interaction and vapor explosions. These processes include single-phase and multi-phase fluid dynamics, thermodynamics and chemical kinetics. The interactions and couplings among these processes have been of particular interest.

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The entropy-inequality work does succeed in obtaining reasonable constraints on constitutive parameters such as virtual mass and pressure-difference coefficients. Based as it is on the averaging of the microscopic entropy inequality, this approach appears to be inappropriate, however, as regards constraints on parameters arising from consideration of velocity fluctuations. Research is continuing in this area, and is related to the model for particle velocity fluctuations discussed below.

Constitutive equations for high Reynolds number flow of a suspension of spheres have been derived. These include such features as virtual mass, lift, a pressure difference force, Reynolds stresses, and an average stress in the particle phase that is not spherical (i. e., not represented as a pressure). The combination of these forces reduces to the force on a single sphere in an accelerating flow, as derived by Taylor.

The model for the evolution of geometry is based on two equations for the evolution of the Gaussian and mean curvatures for a point on a surface. These equations are averaged, and equations for the evolution of volume fraction and interfacial area are derived. The averaged equations for the evolution of geometry include equations for the evolution of volume fraction, interfacial area, Gaussian curvature and mean curvature. these equations are coupled to the mean fields (and consequently, to the mass, momentum, and energy equations) through two fields, the average interfacial (transport) velocity, and the average interfacial normal velocity.

Classical statistical mechanics treats a set of spheres, energized and colliding, as a "gas," and derives expressions for the heat flux and the viscosity. If the particles are in a fluid, a similar model should be possible. Constitutive equations for the interfacial force and the fluid and particle stresses has been derived. This model shows the dependence of these quantities on the particle stress and heat flux. An equation for the evolution of the particle kinetic energy has also been derived. This model needs expressions for the heat flux and stress for the particle phase. One option is to use those derived by researchers in granular flow. Research in this area is continuing.

Research in transition to detonation, say behind a precursor shock, has revealed an interesting sequence of events. It appears that the detonation starts as a constant-volume explosion in a hot-spot, or reaction center, from which a high-velocity reaction wave emerges. This wave, which is supersonic even relative to the flow behind it, has a quasisteady weak-detonation structure. As the wave advances into the preconditioned explosive it decelerates, eventually reaching the Chapman-Jouguet speed. At this point, a weak shock is born at the rear of the reaction zone. This shock quickly advances to the front of the wave, strengthening as it does so, eventually imparting the wave the conventional, ZND structure.

It is also found that transition scenarios can vary significantly, depending upon the constitutive model chosen to represent the explosive material. The events described above take place if the

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explosive is modelled as an ideal gas with a one-step, large activation energy kinetics. Changes in the kinetic scheme and the equation of state may lead to an entirely different picture; for example, the supersonic reaction wave emerging from the hot spot may well have a subsonic character. Current research activity is aimed at achieving a complete classification of the various possibilities.

Much of past research on flame-acoustic interaction was aimed at the acoustics itself, with the flame playing the role of an energy supply. In our work we have emphasized the effect of the applied disturbances on the flame, with special attention to the possibility of extinction caused by gasdynamic disturbances. Fully one-half of Ledder's thesis is devoted to this problem. We find, in particular, that if the time scale of the applied disturbance is fast enough, the flame responds not so much to the amplitude of the disturbance as to the rate at which the amplitude changes. As a result, only a small amount of pressure drop is found to be sufficient to extinguish the flame, provided the pressure is dropped fast enough.

Many industrial accidents are caused by the inadvertent dropping of extremely hot (even molten) metal into a liquid, which then undergoes rapid vaporization – a vapor explosion. We have initiated a study of this problem (the second-half of Ledder's thesis). Through a careful scaling of the problem, which involves a large number of parameter groupings, we have been able to identify those which take on extreme values, thus providing the basis for a rational asymptotic analysis. Such an analysis has been carried out for a specific situation to determine, in particular, the rate of growth of the vapor bubble. Further work, which would take into account the occurence of chemical reactions at the liquid-metal interface, is contemplated.

Personnel supported under this contract

D. A. Drew, who performed most of the multiphase flow research;

A. K. Kapila, who performed most of the reacting flows research;

T. L. Jackson, who collaborated on research in supersonic combustion;

S. Passman, who collaborated on a study of viscous models.

Student supported by the contract

G. Ledder, Ph.D. (1990), now an assistant professor at the University of Nebraska.

Publications under the contract

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5. D. A. Drew, "Stress in the particle phase in a particle-fluid model."

6. D. A. Drew, "Effect of particle velocity fluctuations on inertia coupling."

7. S. L. Passman and D. A. Drew, "Effect of Viscosities in particle- fluid shear flows."